NISTIR 6890

Fire Resistance Determination and Performance Prediction Research Needs Workshop: Proceedings

William Grosshandler
Editor

National Institute of Standards and Technology
Technology Administration, U.S. Department of Commerce

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U.S. Department of Commerce
Donald L. Evans, Secretary

Technology Administration
Phillip J. Bond, Under Secretary of Commerce for Technology

National Institute of Standards and Technology
Arden L. Bement, Jr., Director

E. Simulation of Accidental Fires and Explosions

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Center for the Simulation of Accidental Fires and Explosions

Adel F. Sarofim and Philip J. Smith
Department of Chemical and Fuels Engineering
University of Utah

Workshop on

RESEARCH NEEDS FOR FIRE RESISTANCE DETERMINATION AND PERFORMANCE PREDICTION

NIST Gaithersburg
February 19, 2002

OUTLINE

- Background on C-SAFE
  - What is C-SAFE?
  - Relevance to Workshop
    - *Interdisciplinary*
    - *Large Scale Simulations*
    - *Multi-phase, Multi-scale*
- Vignettes
  - Computational Chemistry
  - Fire Spread
  - Material Point Methods
- Lessons Learned
  - Keys to success
  - Problem areas
- Conclusions

ASCI & C-SAFE

The Accelerated Strategic Computing Initiative (ASCI) Alliances have been set up to develop unclassified simulation science in support of the DOE Defense Program Laboratories mission to safeguard the U.S. nuclear stockpile. Five universities have been funded as part of the ASCI alliance:

Stanford University: development of technology suitable for the design of gas turbine engines

California Institute of Technology: shock waves induced by high explosives on various materials in different phases

University of Chicago: long-standing problem of astrophysical thermonuclear flashes

University of Utah: science-based tools for numerical simulation of accidental fires and explosions, within the context of handling and storing highly flammable material (C-SAFE's project)

University of Illinois: whole-system simulation of solid propellant rockets under both normal and abnormal operating conditions.

Specific Focus

Container

- Metal construction
- Arbitrary size/shape
- Arbitrary location

Hydrocarbon Fire

- Arbitrary Size
- Includes soot

HE Material

- PBX 9501

C-SAFE Team Structure

All-SDRM Step Teams

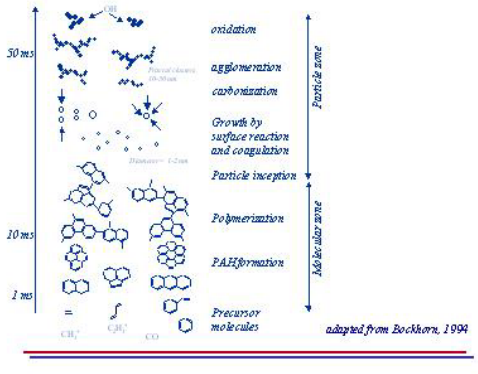
Computer Science
Leaders: Tom Henderson; Steve Parker - SA
Software Engineer: Davison de St. Germain
Key Participants: Chris Johnson, Chuck Hansen, Gary Lindstrom, Kris Sikorski

Ignition	Fire Spread	Container Dynamics	High Energy Transformations	Accidental Detonation
Leader:	Phil Smith	Pat McMurtry	Chuck Wight	
Software Engineer:	Rajesh Rawat	John Schmidt	M. Ovchinnikov	SDRM-specific Step Teams
Key Participants:	Thanh Truong Adel Sarofim Homer Walker	Dan Adams John Nairn Jeff Weiss Grant Smith	Greg Voth Thanh Truong Jack Simons Grant Smith Merrill Beckstead	

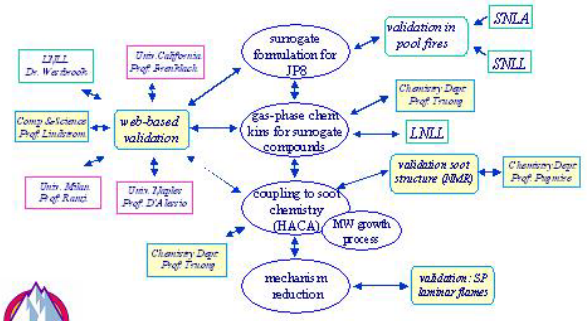
Validation
Leaders: Adel Sarofim, Eric Eddings
Key Participants: Ron Pugmire, Thiokol

Firespread

Soot formation submodel

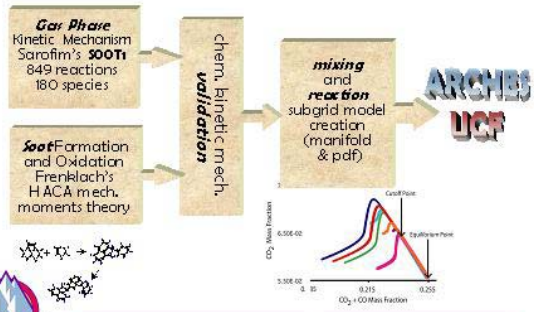


Present Collaborations and Linkages



Chemistry / Mixing & Fire

bridging micro to macro scales in fire simulations



Example: buoyancy driven flames (10m heptane pool fire)

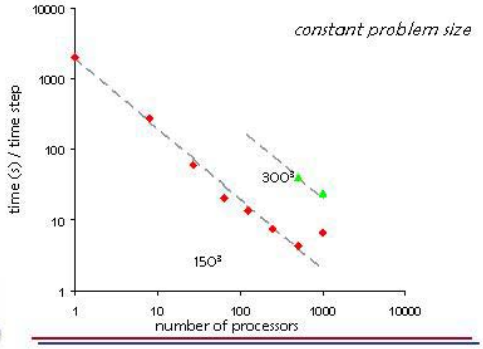
- resolution: 150^3
- domain: $(50m)^3$
- 500 processors
- 18 hrs on Nirvana (LANL)
- 6828 time steps

Jet-Fuel Pool Fire Testing

Jet Fuel pool fire experiments are conducted for comparison with detailed computer models being developed in the Center for Simulation of Accidental Fires and Explosions at the University of Utah

Computer simulation graphic courtesy of Prof. Philip J. Smith, and the Scientific Computing and Imaging (SCI) Institute

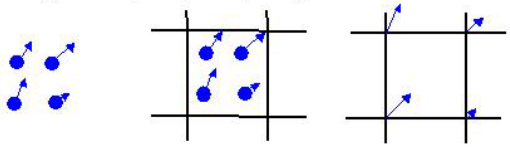
Multiprocessor Scalability



Container Dynamics

The Material Point Method (MPM)

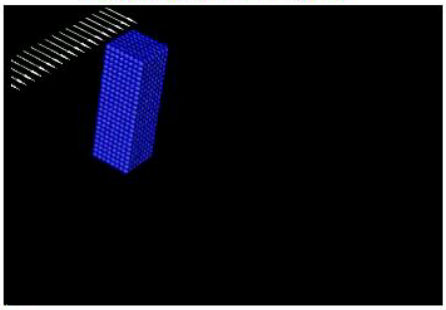
Explicit Algorithm (Sulsky et al., 1994)



1. Lagrangian material points carry all state data
2. Overlying mesh defined
3. Mass,momentum, velocity, stress interpolated to overlying mesh. Interpolation conserves mass, momentum

MPM Demonstration

Flexible beam in a crossflow



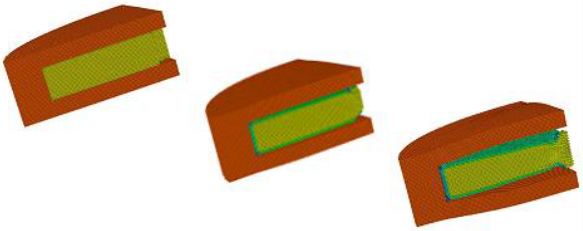
HIGH ENERGY MATERIALS

Container/PBX Heating Response Simulation

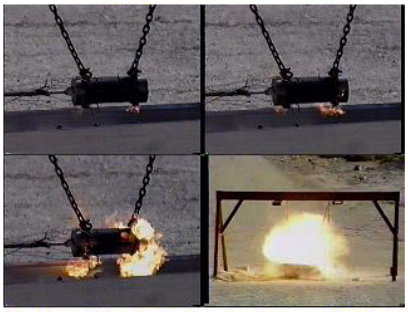
Container: Steel
bulk modulus: 200e9 Pa
shear modulus: 77.8e9 Pa
yield stress: 250e6 Pa
hardening modulus: 77e7 Pa
OD: 0.03136 m
ID: 0.02496 m
Thickness: 0.0016 m
Contents: PBX – ViscoScram
Center hole: 0.0032 m
Burn Model: HE Team, rate =Akp^n
Initial Temperature: PBX, 300K
Specified heat flux at container surface

Container/PBX Heating Response Simulation

Mass evolution:

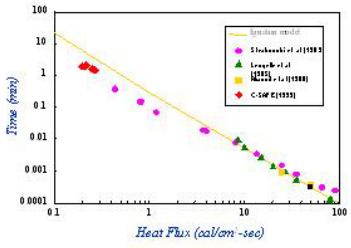


Images from Propane-Fired Fast-Cook Off Test



(a), (b) and (c) Release of pyrolysis gases; (d)Explosion

Time to Explosion Correlates with Heat Flux (Inferred from T-t using Duhammel Superposition)

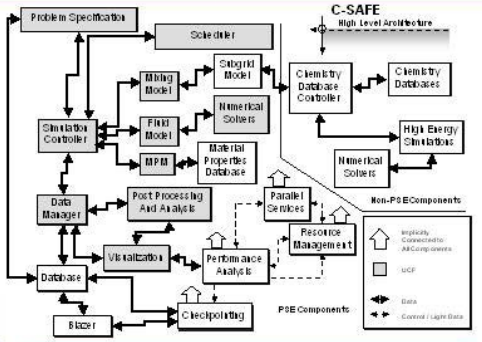


Container Remnants

Electrical Input:
110 V - 19 kW/m^2
Time to Explosion:
26 min

Electrical Input:
220 V - 83 kW/m^2
Time to Explosion:
3 min

Uintah Computational Framework



Keys to Success

- Well-defined goals
- Management Committee chaired by Dave Pershing to provide
  - priorities,
  - timetable,
  - resource allocation,
  - conflict resolution
- Designation of software engineer for each step to work with the computer scientists on
  - Algorithm development
  - Common computer architecture
  - Problem solving environment
  - Parellelization, Vizualization
- Networking with the DOE laboratories and with national and other discipline experts
- Tie in with experimental programs for validation

Problem Areas

- Interfaces
  - Between phases
- Communication
  - Between disciplines
  - With ultimate user
- Data
  - Communication
  - Storage
  - Mining

Conclusions

- Crosscutting Issues need Interdisciplinary Approaches
  - C-SAFE experience underlines importance of close collaboration between software engineers and computer scientists
  - 'Amphibians' needed to bridge gaps between disciplines
  - Importance of communication cannot be overstated (GBS: "The greatest myth about communication is the mistaken belief that it has taken place.")
- Major Advances in Simulation Science
  - Computational chemistry for properties, mechanisms, kinetics
  - More detailed kinetic and fluid mechanics models can be included in massively parallel computations
  - Material point methods show promise for handling large deformations and break up of structures
  - Experimental validation and guidance is crucial